Introduction to Machine Learning

Measures of Accuracy

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Outline

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What did we see until now?

The design of learning machines from two main points:

- Statistical Point of View
- Linear Algebra and Optimization Point of View

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$$\mathcal{D} = \{(x_i, y_i) | i = 1, 2, ..., N\} \quad (1)$$

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Our Final Equation

$$E_D\left(\left(g\left(\boldsymbol{x}|\mathcal{D}\right)-E\left[y|\boldsymbol{x}\right]\right)^2\right)=\underbrace{E_D\left(\left(g\left(\boldsymbol{x}|\mathcal{D}\right)-E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right]\right)^2\right)}_{VARIANCE}+\underbrace{\left(E_D\left[g\left(\boldsymbol{x}|\mathcal{D}\right)\right]-E\left[y|\boldsymbol{x}\right]\right)^2}_{BIAS}$$

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Assume

The data is generated by the following function

$$y = f(x) + \epsilon,$$
$$\epsilon \sim \mathcal{N}\left(0, \sigma_\epsilon^2\right)$$

We know that

The optimum regressor is $E[y|x] = f(x)$

Furthermore

Assume that the randomness in the different training sets, $\mathcal{D}$, is due to the y_i's (Affected by noise), while the respective points, x_i, are fixed.

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Sampling the Space

Imagine that $\mathcal{D} \subset [x_1, x_2]$ in which x lies

For example, you can choose $x_i = x_1 + \frac{x_2 - x_1}{N-1}(i-1)$ with $i = 1, 2, ..., N$

Case 1

Choose the estimate of $f(x)$, $g(x|\mathcal{D})$, to be independent of $\mathcal{D}$

For example, $g(x) = w_1 x + w_0$

For example, the points are spread around $(x, f(x))$

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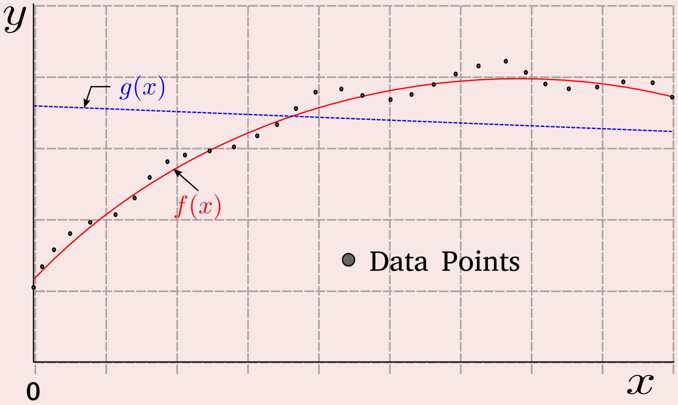

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Now, $g_1(x)$ corresponds to a polynomial of high degree so it can pass through each training point in $\mathcal{D}$.

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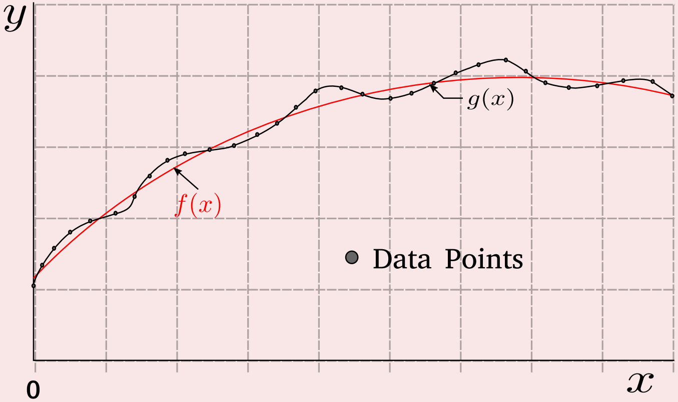

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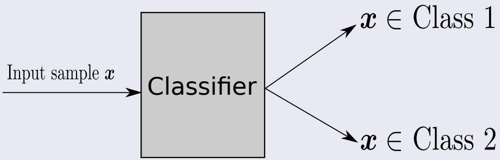
Sooner of Latter you need to know how efficient is your algorithm

Thus, we need a measures of accuracy

Thus, we begin with the classic classifier for two classes



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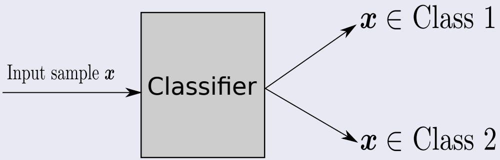

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For this, we can use the idea of error in statistics.

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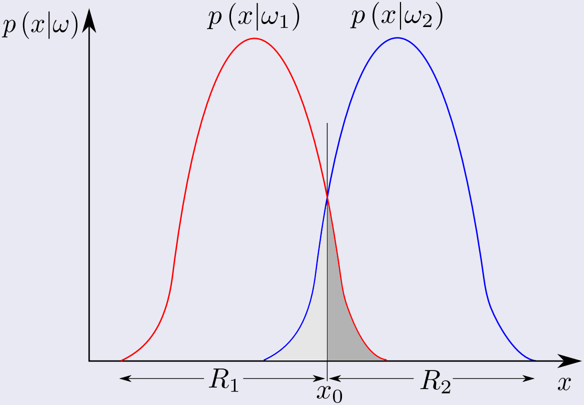

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α error

Definition (Type I Error - False Positive)

α is the probability that the test will lead to the rejection of the hypothesis H_0 when that hypothesis is true.

- You have a device that fails $\alpha = 0.05$ meaning that it fails 5% of the time
- This says that you ha low chance of a wrong circuit

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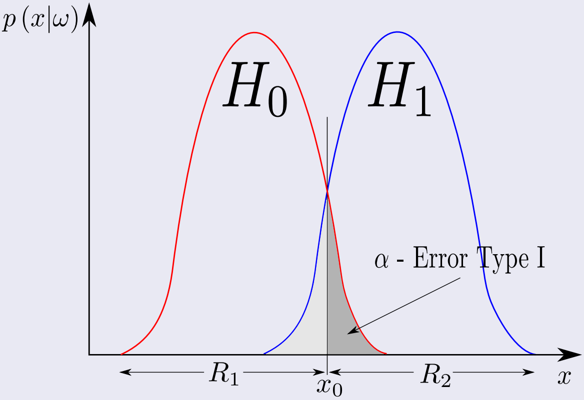

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This can be seen as a table

Confusion Matrix from the statistic point of view

Table of error types		Null Hypothesis H_0	
		True	False
Decision about H_0	Reject	Type I Error - α **False Positive**	Correct Inference **True Positive**
	Fail to reject	Correct Inference **True Negative**	Type II Error - β **False Negative**

In the case of two classes, we have

Confusion Matrix from the Machine Learning point of view

		Actual Class	
		Positive	Negative
Predicted Classes	Positive	**True Positive (TP)**	**False Positives (FP)**
	Negative	**False Negatives (FN)**	**True Negatives (TN)**

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Accuracy

Definition

The proportion of getting correct classification of the Positive and Negative classes.

Thus

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + FN + TN}$$

Problem - accuracy assumes equal cost for both kinds of errors

Is 99% accuracy good, bad or terrible? It depends on the problem.

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Specificity

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We can do better than these simple measures of accuracy

Given these initial measures of validity

it is possible to obtain a more precise model evaluation, the ROC curves.

The ROC Curves plot

It is a model-wide evaluation measure that is based on two basic evaluation measures:

1. **Specificity** is a performance measure of the whole negative part of a dataset.
2. **Sensitivity** is a performance measure of the whole positive part.

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What the ROC Curves uses

We have a plot where

The ROC plot uses specificity on the x-axis and sensitivity on the y-axis.

1. Two adjacent ROC points can be connected by a straight line
2. The curve starts at (0.0, 0.0) and ends at (1.0, 1.0)

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False Positive Rate (FPR) is identical with specificity, and True Positive Rate (TPR) is identical with sensitivity.

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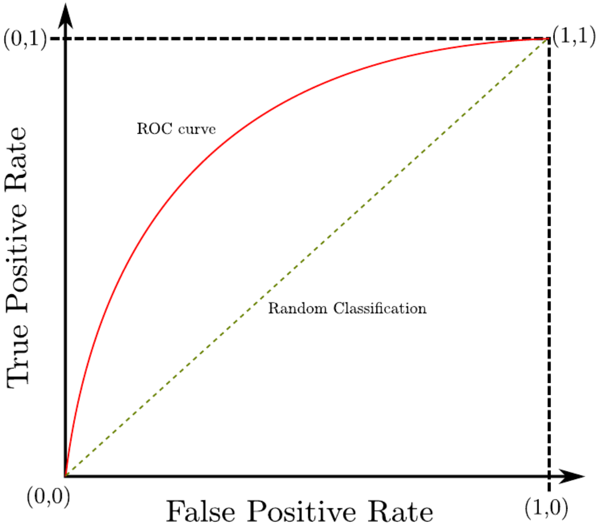

(0,1)
(1,1)
ROC curve
Random Classification
True Positive Rate
(0,0)
False Positive Rate
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Algorithm ROC point generation

Input: L, the set of test examples; $f(i)$, the probabilistic classifier estimate that example i is positive; P and N, the number of positive and negative examples.

Ouput: R, a list of ROC points increasing by false positive rate.

1. $L_{sorted} \leftarrow L$ sorted decreasing by f scores
2. $FP \leftarrow TP \leftarrow 0; R \leftarrow \langle\rangle; fprev \leftarrow -\infty; i \leftarrow 1$
3. **while** $i \leq |L_{sorted}|$
4.   **if** $f(i) \neq f_{prev}$ **then**
5. $R.append\left(\frac{FP}{N}, \frac{TP}{P}\right)$
6. $fprev \leftarrow f(i)$
7.   **if** L_{sorted} is a positive example **then** $TP = TP + 1$
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A Partial List is

1. Area Under the Curve (AUC)
2. Equal Error Rate (EER)
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A Simple Definition

We have

$$AUC = \int ROC\left(p\right)dp = \sum_{i=1}^{N} ROC\left(f\left(\frac{1}{i}\right)\right)\left[\frac{i}{N} - \frac{i-1}{N}\right]$$

This equation has the following meaning

- The probability that a randomly selected observation X from the **positive class** would have a higher score than a randomly selected observation Y from the **negative class.**

$$P\left(X > Y\right)$$

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The AUC gives the mean **true positive** rate averaged uniformly across the **false positive** rate.

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What we want

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- A quality measure to measure different classifiers (for different parameter values).

We call that as

$$R(f) = E_{\mathcal{D}}\left[L\left(y, f\left(x\right)\right)\right]. \quad (2)$$

Example: $L\left(y, f\left(x\right)\right) = \left\|y - f\left(x\right)\right\|_2^2$

More precisely

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- We use the validation set to estimate

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- Re-train the classifier with the best parameter γ^* on all data except the test set (i.e. train + validation data).
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Procedure

To estimate the risk of a classifier f:

1. Split data into K equally sized parts (called "folds").
2. Train an instance f_k of the classifier, using all folds except fold k as training data.
3. Compute the cross validation (CV) estimate:

$$\hat{R}_{CV}\left(f\left(x|\gamma_i\right)\right) = \frac{1}{N_v}\sum_{i=1}^{N_v} L\left(y_i f\left(x_{k(i)}|\gamma_j\right)\right) \tag{4}$$

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$K = 5$

- Randomize the data and split the data in five folds

Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
1	2	3	4	5

- Then select one fold for testing

Therefore

- Cross validation procedure does not involve the test data.

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Train Data + Validation Data	Test

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